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*Title:* INTEGRATING LINEAR INTERPOLATION FUNCTIONS ACROSS TWO AND THREE-DIMENSIONAL CELL BOUNDARIES


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# Integrating Linear Interpolation Functions Across Two- and Three-Dimensional Cell Boundaries

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## Objective

Develop *discrete expansions* for linear interpolation functions: expansions that are similar to a multivariable Taylor's series but — by accounting for discontinuous interpolation derivatives across cell boundaries — are valid throughout a discretized domain.

## Particle Methods

Particle methods — computational models of particle dynamics — often use interpolation functions to gather and scatter data between particles and discretized continuum fields. These models require a series expansion of the interpolation function for two purposes:

- numerical analyses used to establish the models' consistency and accuracy
- logical-coordinate evaluation used to locate particles within a grid system.

Existing expansions (truncated, single-variable Taylor's series) are inherently invalid for expansions that extend across cell boundaries where interpolation derivatives are generally discontinuous.

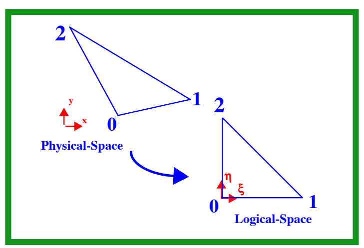
## Linear Interpolation

Used for both data interpolation and coordinate transformation — from physical space $\bar{X} = (x, y, z)^T$ to logical space $\bar{\xi} = (\xi, \eta, \zeta)^T$ coordinates — within discretized domains that include 2-D triangles and 3-D tetrahedrals.

$$\bar{X}\left(\bar{\xi}, \bar{X}^{cv}\right) = (1 - \xi - \eta - \zeta)\ {}^{0}\bar{X} + (\xi)\ {}^{1}\bar{X} + (\eta)\ {}^{2}\bar{X} + (\zeta)\ {}^{3}\bar{X}$$

Bound logical coordinates: $\xi \geq 0$, $\eta \geq 0$, $\zeta \geq 0$, and $\xi + \eta + \zeta \leq 1$

Cell-vertex (cv) coordinate vector: $\bar{X}^{cv} = \left({}^{0}\bar{X}, {}^{1}\bar{X}, {}^{2}\bar{X}, {}^{3}\bar{X}\right)^T$




## Discrete Expansions for Linear Interpolation

### Total Differential

Total differential: a relationship between infinitesimal changes of the physical, logical, and cell-vertex coordinates $d\bar{X} = f\left(d\bar{\xi}, d\bar{X}^{cv}\right)$:

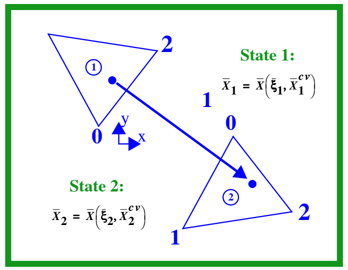
$$d\bar{X} = \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}^{cv}\right) d\bar{\xi} + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi})\, d\bar{X}^{cv}$$

Discrete-expansion: a relationship between the finite changes of these coordinates: $\Delta\bar{X} = f\left(\Delta\bar{\xi}, \Delta\bar{X}^{cv}\right)$.

We integrate the total-differential between two particles located in separate, noncontiguous grid cells: State 1 and State 2.

$$\int_1^2 d\bar{X} = \int_1^2 \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}^{cv}\right) d\bar{\xi} + \int_1^2 \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi})\, d\bar{X}^{cv}$$

Interpolation derivatives are generally not continuous across cell boundaries; original total-differential is not valid.




### Parameterization

Parameterize integration coordinate-space $\left(\bar{\xi}, \bar{X}^{cv}\right)$ with the variable 's', where $0 \leq s \leq 1$, using a linear technique: $\phi(s) = (1-s)\ \phi_1 + (s)\ \phi_2$.

$$\int_0^1 \frac{\partial \bar{X}(s)}{\partial s}\, ds = \int_0^1 \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}^{cv}(s)\right) \frac{\partial \bar{\xi}(s)}{\partial s}\, ds + \int_0^1 \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}(s)) \frac{\partial \bar{X}^{cv}(s)}{\partial s}\, ds$$

Parameterized interpolation derivatives are continuous across cell boundaries; parameterized total differential is valid.

### Direct Integration Pathline

A straight or direct line between particle State 1 and State 2.

$$\Delta\bar{X} = \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\hat{\bar{X}}^{cv}\right) \Delta\bar{\xi} + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}\left(\hat{\bar{\xi}}\right) \Delta\bar{X}^{cv}$$

Finite-difference vectors: $\Delta\bar{X} = \bar{X}_2 - \bar{X}_1$, $\Delta\bar{\xi} = \bar{\xi}_2 - \bar{\xi}_1$, and $\Delta\bar{X}^{cv} = \bar{X}_2^{cv} - \bar{X}_1^{cv}$.

Particle end-state averages: $\hat{\bar{\xi}} = (\bar{\xi}_1 + \bar{\xi}_2)/2$ and $\hat{\bar{X}}^{cv} = \left(\bar{X}_1^{cv} + \bar{X}_2^{cv}\right)/2$.

### Upper-Step Integration Pathline

Partition the integration pathline in the $\left(\bar{\xi}, \bar{X}^{cv}\right)$ plane.
Integrate the upper-step pathline from State 1 to State A to State 2.

$$\Delta\bar{X} = \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}_2^{cv}\right) \Delta\bar{\xi} + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}_1)\ \Delta\bar{X}^{cv}$$

### Lower-Step Integration Pathline

Partition the integration pathline in the $\left(\bar{\xi}, \bar{X}^{cv}\right)$ plane.
Integrate the lower-step pathline from State 1 to State B to State 2.

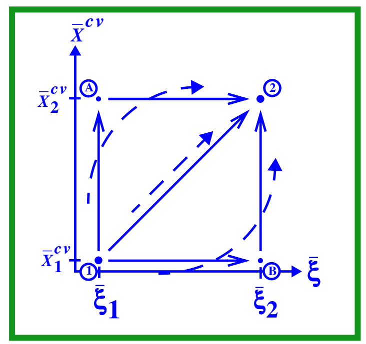
$$\Delta\bar{X} = \frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}_1^{cv}\right) \Delta\bar{\xi} + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}_2)\ \Delta\bar{X}^{cv}$$

Upper-step and lower-step discrete expansions are mirror images.

Identical results for 2-D and 3-D linear-interpolation discrete expansions.

Discrete expansions acknowledge the full functional dependence of interpolation and inherently account for discontinuities across cell boundaries.

The total-differential method is a general solution technique for developing interpolation discrete expansions.




## Numerical Analysis

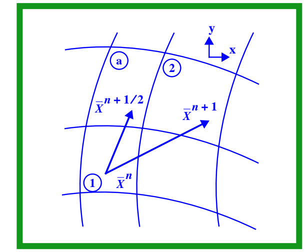
Analytical investigation of particle methods is used to establish the method's mathematical consistency and numerical accuracy.

Example: Predictor-Corrector time-integration for $d\bar{X}/dt = \bar{V}(\bar{X}, t)$.

Discrete expansions are required to relate interpolated velocities at State A to State 1:

$$\bar{V}\left(\bar{\xi}_a, \bar{V}_a^{cv}\right) = \bar{V}\left(\bar{\xi}_1, \bar{V}_1^{cv}\right) + \frac{\partial \bar{V}}{\partial \bar{\xi}}\left(\bar{V}_a^{cv}\right) \Delta\bar{\xi} + \frac{\partial \bar{V}}{\partial \bar{V}^{cv}}(\bar{\xi}_1)\ \Delta\bar{V}^{cv}$$

For computational models that use interpolation, discrete expansions represent a key advancement in the capability to analyze existing models and to develop advanced models.




## Logical-Coordinate Evaluation

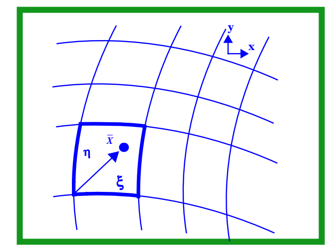
Spatial transformation of a particle-position vector from global, physical space $\bar{X}$ to a local, cell-based coordinate system $\bar{\xi}$.

Discrete expansions are required to relate the known $\Delta\bar{X}$ to unknown $\Delta\bar{\xi}$.

$$\frac{\partial \bar{X}}{\partial \bar{\xi}}\left(\bar{X}_2^{cv}\right) \Delta\bar{\xi} = (\bar{X}_2 - \bar{X}_1) - \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}_1)\ \Delta\bar{X}^{cv}$$

Solution characteristics:

- algorithmically robust (has a guaranteed nonsingular Jacobian matrix), and
- computationally efficient (derivatives are constant, including the Jacobian matrix).




## Summary

Discrete-expansions represent a key advancement for any particle method that uses interpolation by

- providing the capability to analytically define a method's mathematical consistency and numerical accuracy, and
- representing an algorithmically robust and computationally efficient method to locate particles within a grid.

## Next Development Step

Complete a similar total-differential discrete-expansion analysis for nonlinear interpolation: bilinear and trilinear functions.

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